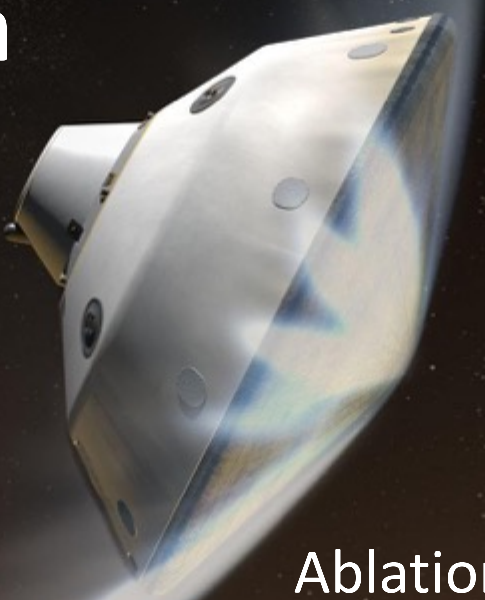
Particle methods for tortuosity factors in porous media



Joseph C. Ferguson [1]
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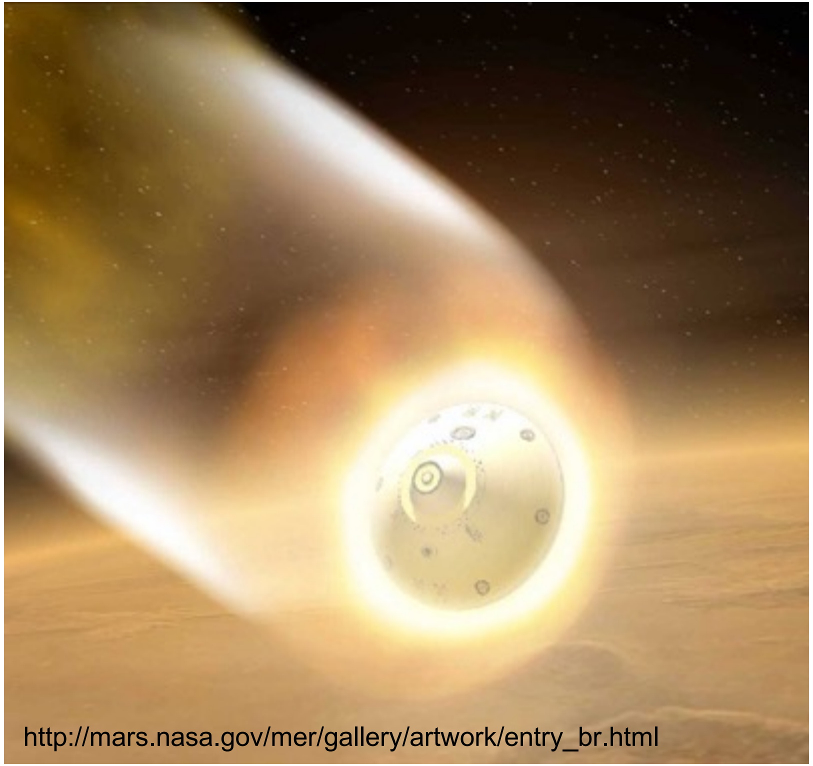
1. Science and Technology Corp. at NASA Ames Research Center
2. Analytical Mechanical Associates Inc. at NASA Ames Research Center
3. Advanced Supercomputing Division, NASA Ames Research Center

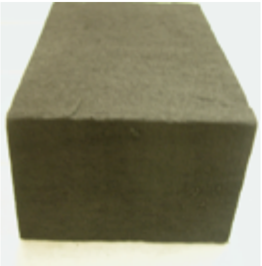
Ablation WS, 2017
Bozeman, MT

Ablative Thermal Protection Systems



Artist rendering of MSL entry

FiberForm®



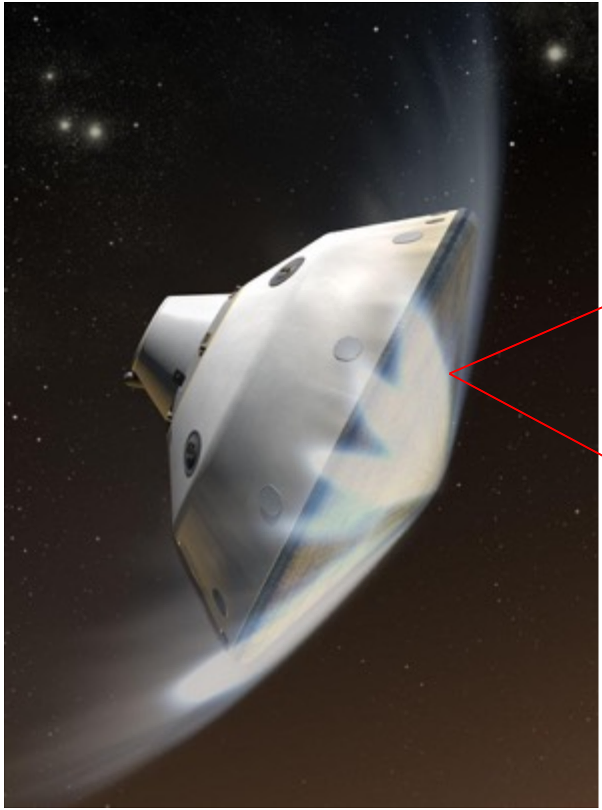
+

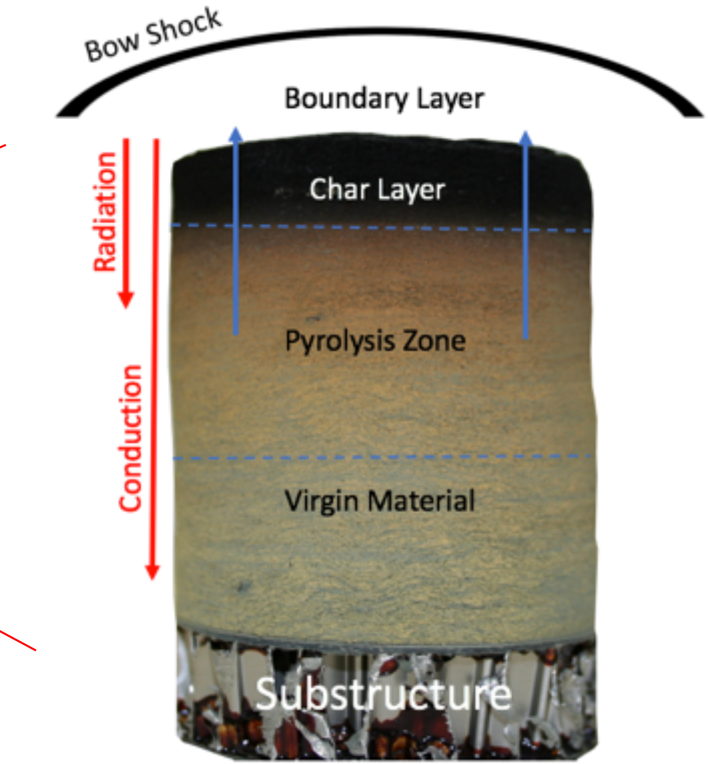
Resin

||

PICA

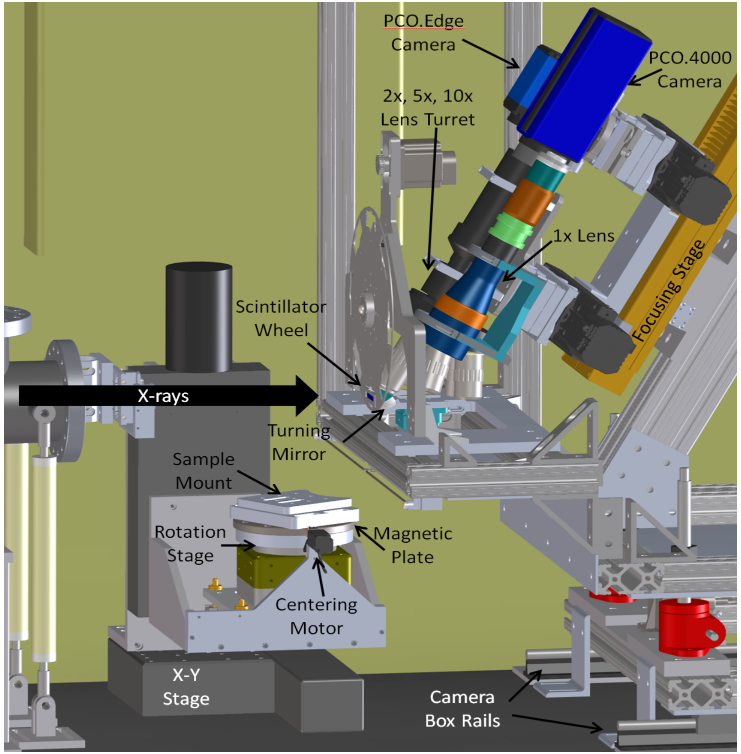
Material Design and Modeling





X-ray micro-tomography

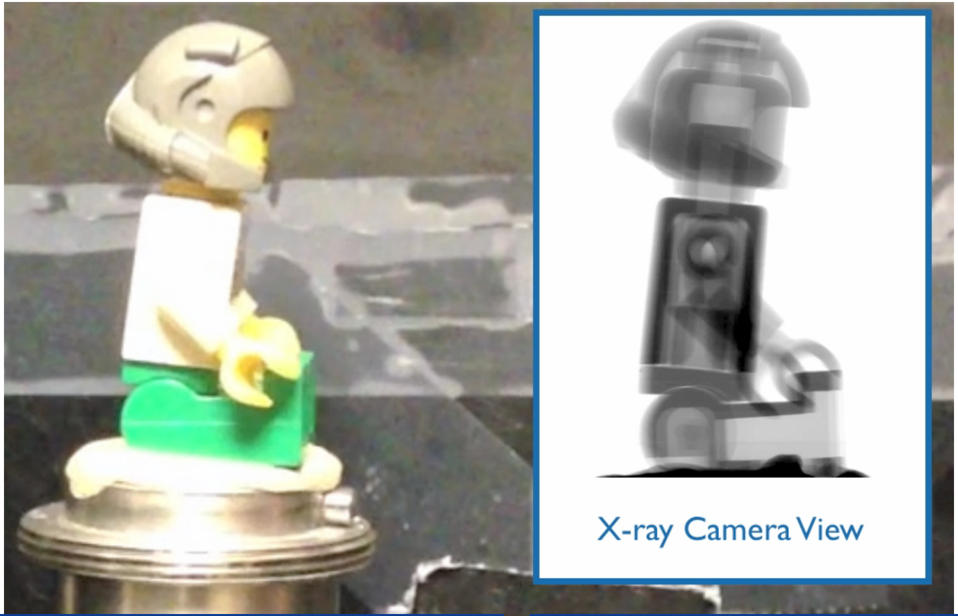
- Advanced Light Source (ALS) at the Lawrence Berkeley Natl. Laboratory
- Synchrotron electron accelerator used to produce 14KeV X-rays
- Used for many research areas, including optics, chemical reaction dynamics, biological imaging, and **X-ray micro-tomography**.



http://www2.lbl.gov/MicroWorlds/ALSTool

X-ray micro-tomography

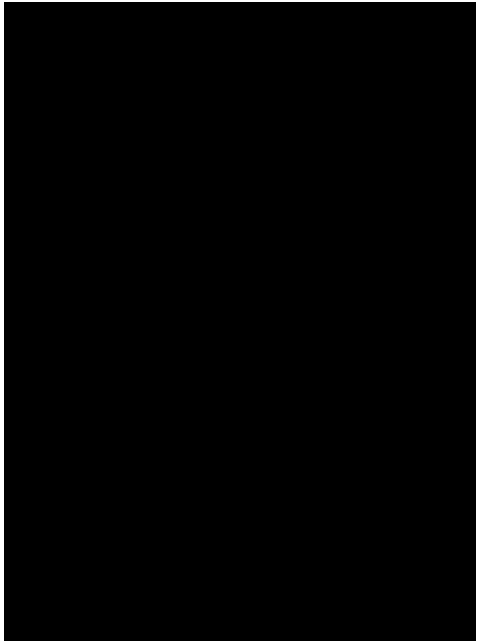
Collect X-ray images of the sample as you rotate it through 180°



Penetrating power

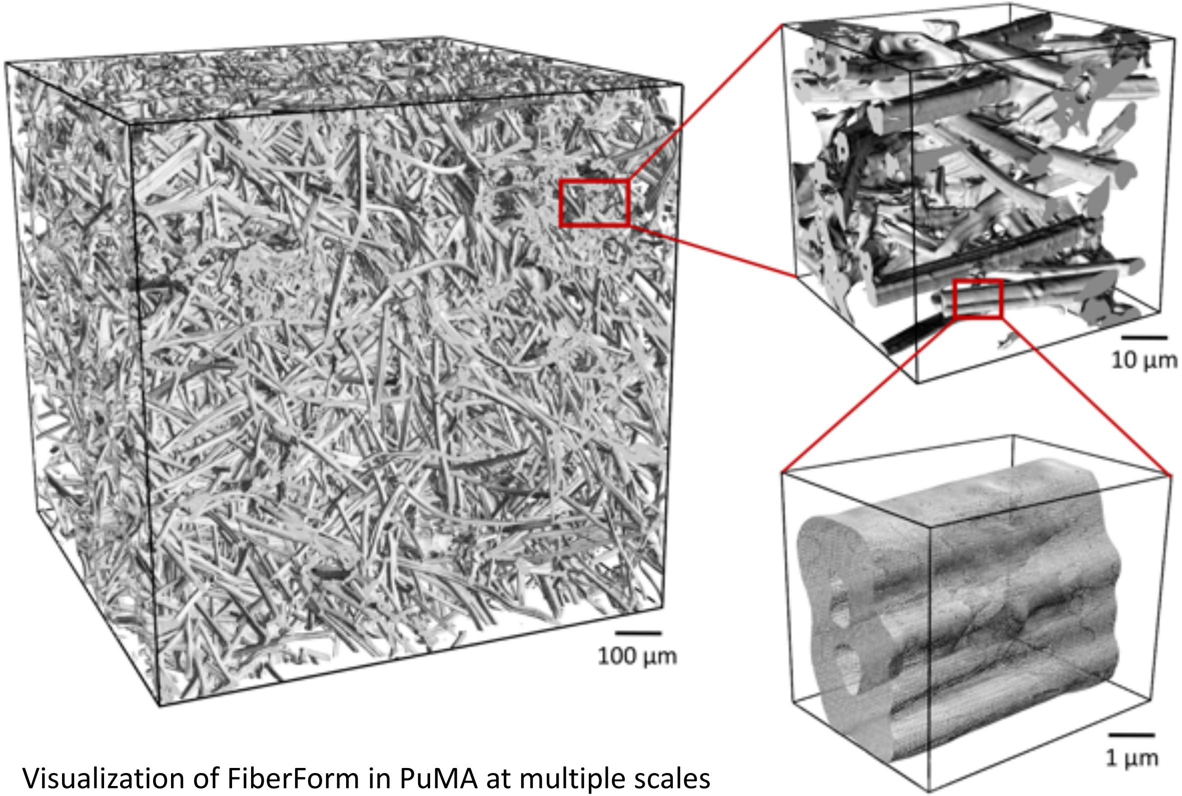
Multiple angles

Use this series of images to "reconstruct" the 3D object



Courtesy of D. Parkinson (ALS)

X-ray micro-tomography



Visualization of FiberForm in PuMA at multiple scales

Porous Materials Analysis (PuMA)

Domain Generation
- Artificial Material Generator
- Micro-tomography Import, Processing, and Thresholding

Visualization
- Marching Cubes
- OpenGL Surface Rendering

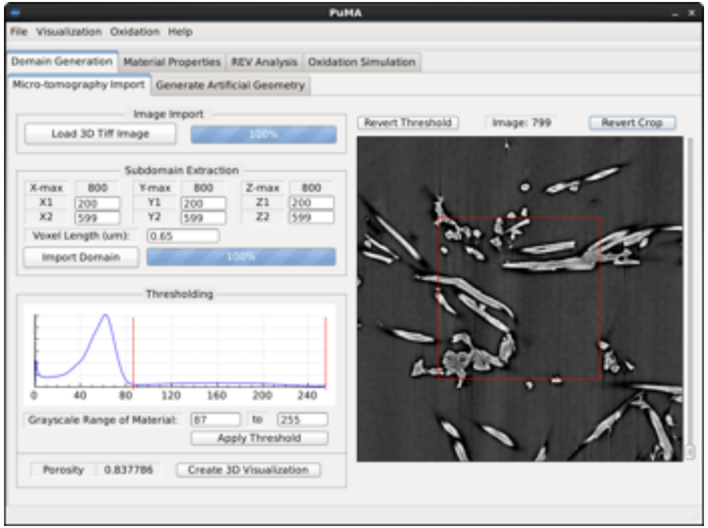
Material Properties
- Porosity
- Specific Surface Area
- Effective Thermal Conductivity
- Effective Electrical Conductivity
- Diffusivity / Tortuosity (Bulk and Knudsen)
- Representative Elementary Volume

Material Response
- Oxidation Simulations
- Transient Heat Transfer *

*Under Development

Technical Specifications

- Written in C++
- GUI built on QT
- Visualization module based on OpenGL
- Parallelized using OpenMP for shared memory systems

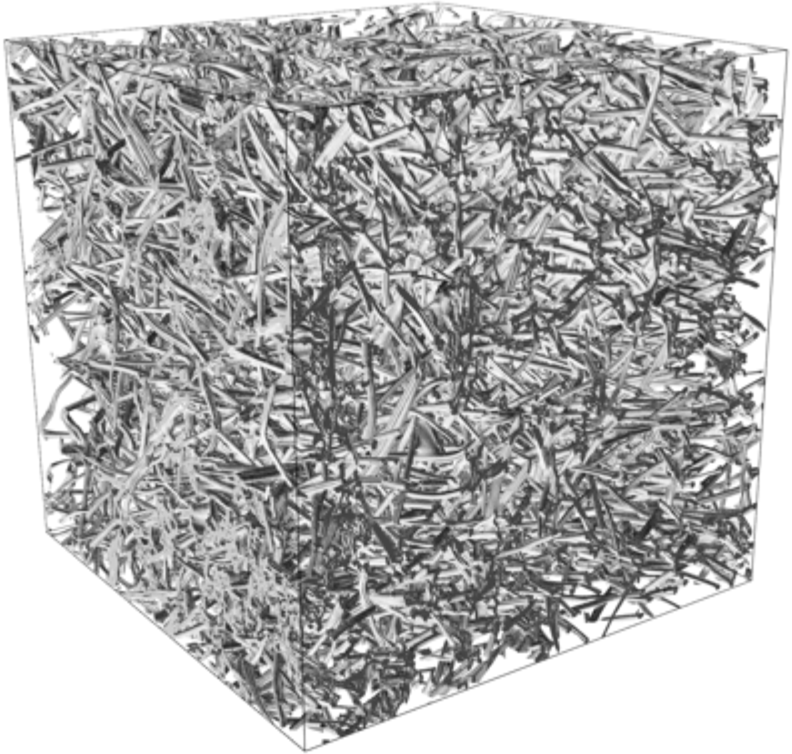


Tortuosity Factors

- Quantifies a materials resistance to a diffusive flux
- Important in modeling diffusion/reaction systems – such as ablative TPS response

$$\eta = \varepsilon \frac{D_{ref}}{D_{eff}}$$

- η = tortuosity factors
- ε = porosity
- D_{ref} = reference diffusion coefficient
- D_{eff} = effective diffusion coefficient



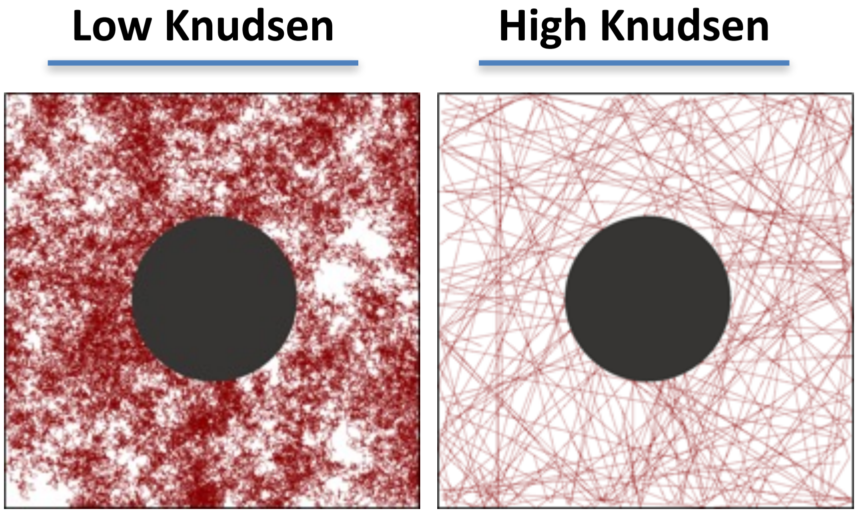
Surface rendering of FiberForm tomography in PuMA V2.1. Visualization contains ≈ 500 million triangles.

Knudsen Number

- Non-dimensional number which defines the diffusion regime

$$\mathrm{Kn} = \frac{\bar{\lambda}}{l_D} = \frac{\text{Mean Free Path}}{\text{Characteristic Length}}$$

- Continuum: Kn << 1
- Transitional: Kn $\approx$ 1
- Rarified: Kn >> 1



2D diffusivity simulations using a random walk method in PuMA. Particle paths are visualized in red.

Tortuosity Factors

- Quantifies a materials resistance to a diffusive flux
- Important in modeling diffusion/reaction systems – such as ablative TPS response

$$\eta = \varepsilon \frac{D_{ref}}{D_{eff}}$$

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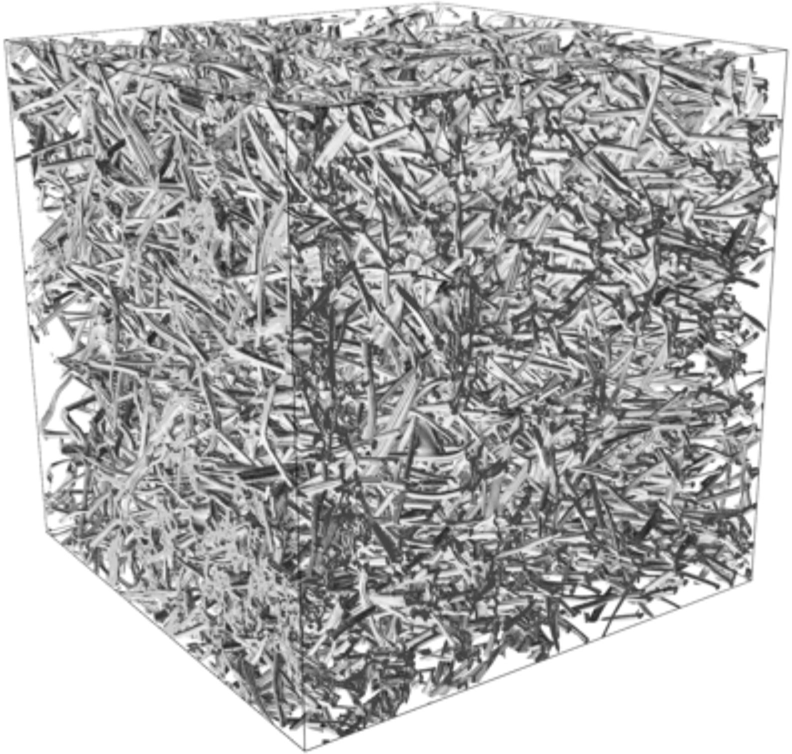


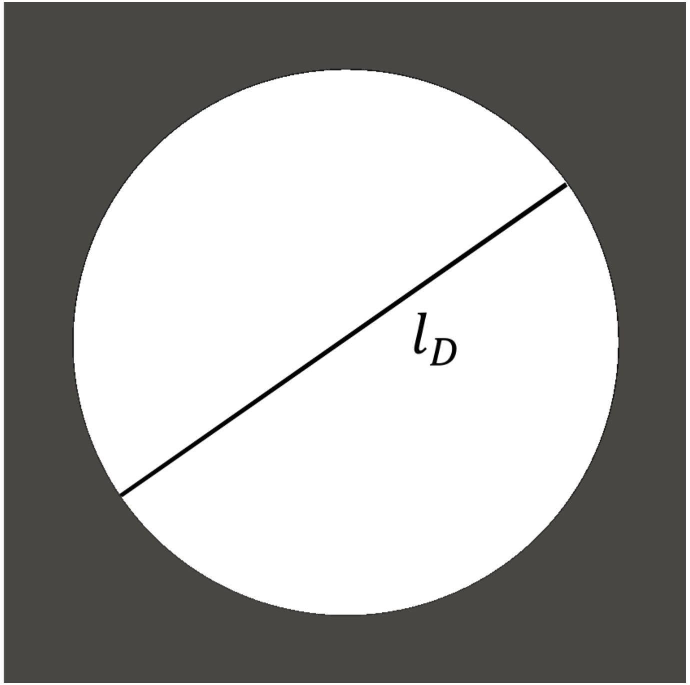
Surface rendering of FiberForm tomography in PuMA V2.1. Visualization contains ≈ 500 million triangles.

Reference Diffusion Coefficient

- D_{ref} = reference diffusion coefficient

Continuum	**Free Molecular**
$D_{ref} = D_{bulk}$	D_{bulk} does not exist

- $D_{bulk} = \frac{1}{3}\bar{v}\bar{\lambda}$, which is undefined as the mean free path approaches infinity
- D_{ref} therefore must be based on a length scale. In this case, the Diffusion coefficient through a capillary of diameter l_D



$\bar{v}$ = mean thermal velocity
$\bar{\lambda}$ = mean free path

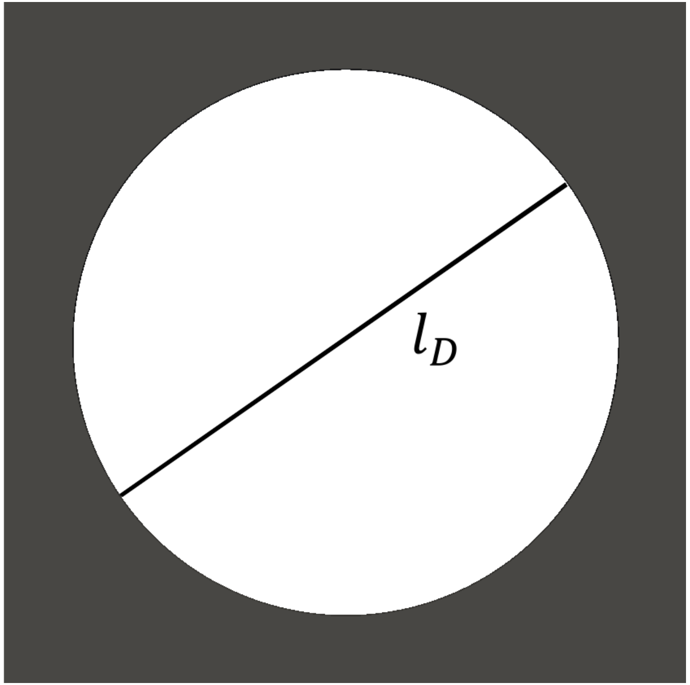
Bosanquet Approximation

- Used to approximate D_{ref} based on known values for D_b and D_k. [1]

$$\frac{1}{D_{ref}} = \frac{1}{D_b} + \frac{1}{D_k}$$

- Rewritten for single species diffusion in a capillary, D_{ref} becomes [2]

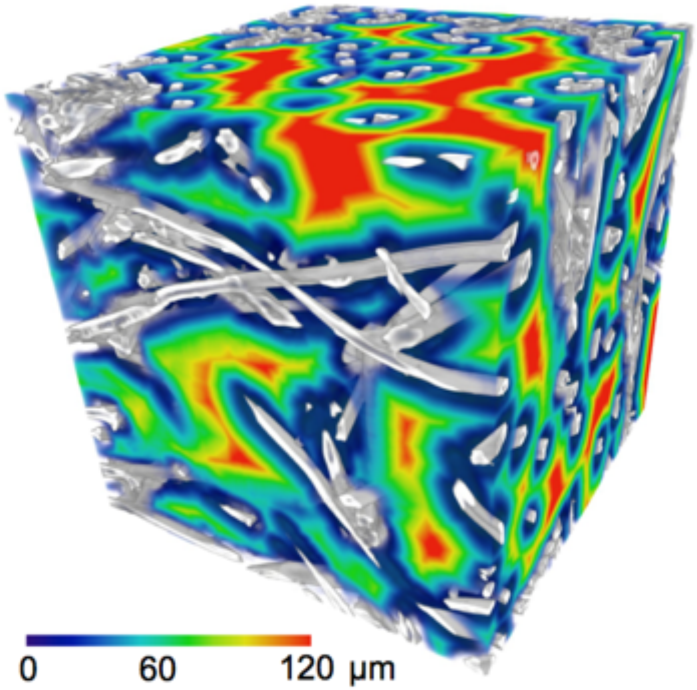
$$D_{ref} = \frac{1}{3}\,\bar{v}\left(\frac{\bar{\lambda}\,l_D}{\bar{\lambda} + \ l_D}\right)$$



[1] Tomadakis, 1998
[2] Pollard, 1948

Choice of Length Scale

1. Define l_D based on an approximate geometric length scale for the material. Typically $\frac{4\varepsilon}{S}$ or mean intercept length. (Tomadakis, Lachaud, Geodict)
2. Define l_D after the simulations are complete as the value which makes the tortuosity factor vs. Knudsen number plot converge to a single value. (Zalc)



Pore size distribution, computed in GeoDict, of FiberForm.

Length Scale Option #1

Define l_D based on an approximate geometric length scale for the material. Typically $\frac{4\varepsilon}{S}$ or mear intercept length. (Tomadakis, Lachaud, Geodict, PuMA)

- Most often used in the literature and software
- Requires values of η_b, η_k and l_D in order to apply the Bosanquet approximation
- η is no longer a purely geometrical property, as it is now a function of the Knudsen numbei
- Since η_b had no physical meaning without l_D, this can produce confusing results of $\eta_k < 1$

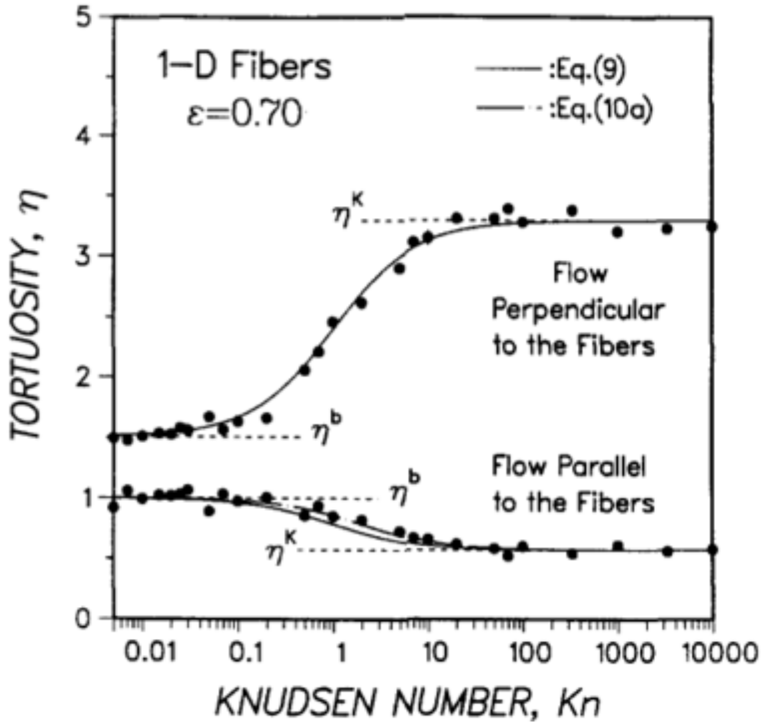
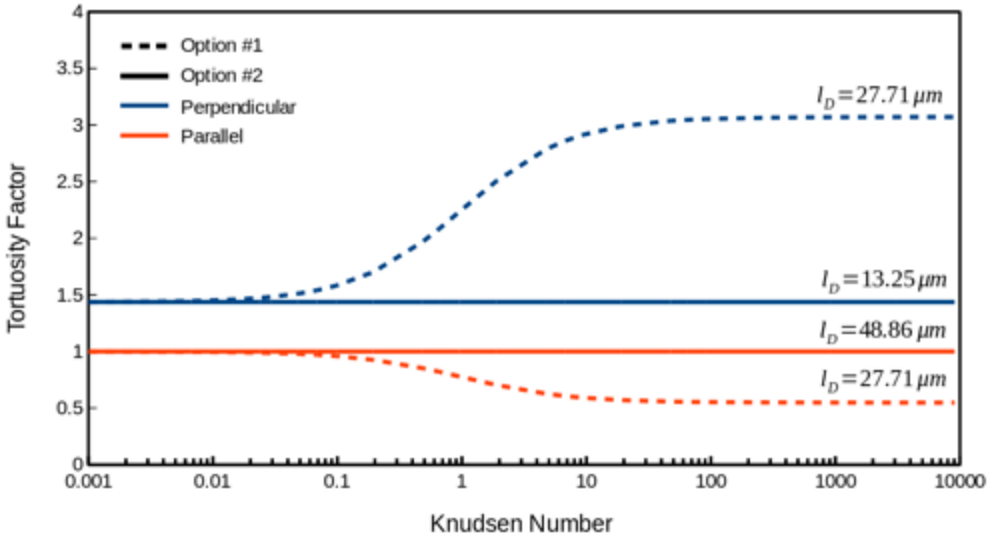


Figure from Tomadakis, 1993

Length Scale Option #2

Define l_D after the simulations are complete as the value which makes the tortuosity vs. Knudsen number plot converge to a single value. (Zalc, PuMA)

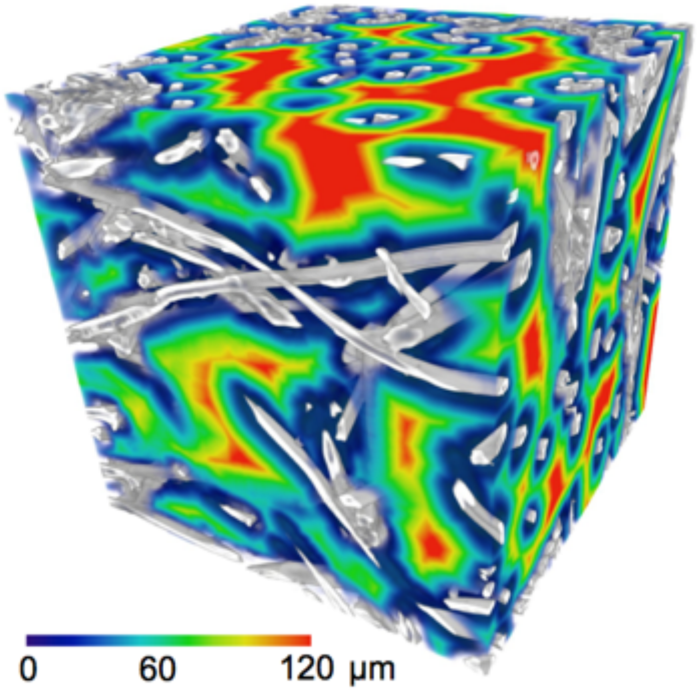
- Requires only one value of η and a computed length scale, l_D, in order to apply the Bosanquet approximation
- η is now longer a purely geometrical property, no longer a function of Kn
- Easier to understand and implement



Tortuosity factor vs Knudsen Number for 1D fibers, computed in PuMA, showing the parallel and perpendicular tortuosity factors for Option #1 and Option #2

Choice of Length Scale

1. Define l_D based on an approximate geometric length scale for the material. Typically $\frac{4\varepsilon}{S}$ or mean intercept length. (Tomadakis, Lachaud, Geodict)
2. **Define l_D after the simulations are complete as the value which makes the tortuosity factor vs. Knudsen number plot converge to a single value. (Zalc)**



Pore size distribution, computed in GeoDict, of FiberForm.

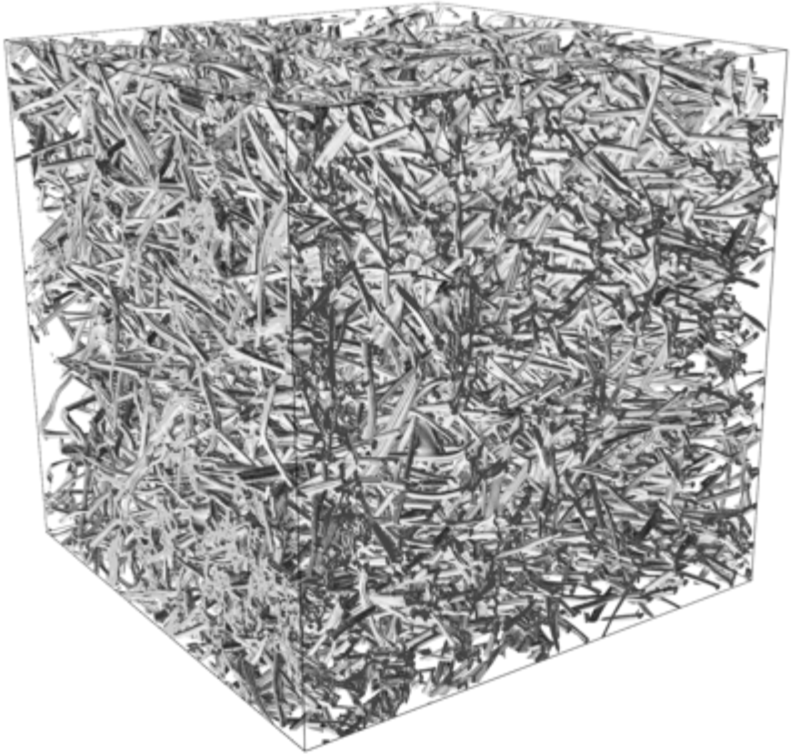
Applying Tortuosity Factors

- Used to compute D_{eff} within a porous media, with known tortuosity factor, η, known length scale, l_D, and known gas properties.

$$D_{eff} = \varepsilon \frac{D_{ref}}{\eta}$$

- Using Bosanquet approximation to approximate D_{ref}, the equation becomes

$$D_{eff} = \frac{\varepsilon}{3\eta} \bar{v} \left(\frac{\bar{\lambda} l_D}{\bar{\lambda} + l_D} \right)$$



Surface rendering of FiberForm tomography in PuMA V2.1. Visualization contains ≈ 500 million triangles.

Numerical Methods

Continuum

- Can be solved using typical numerical methods such as finite volume and finite difference

1. Geodict - Explicit Jump Solver
2. PuMA – Explicit Jump Solver
3. TauFactor – Finite Volume solver

Rarified

- Must be solved using particle methods to account for Knudsen effects

1. PuMA – Random walk solver
2. Geodict – Random walk solver (Knudsen regime)
3. SPARTA – Direct Simulation Monte Carlo

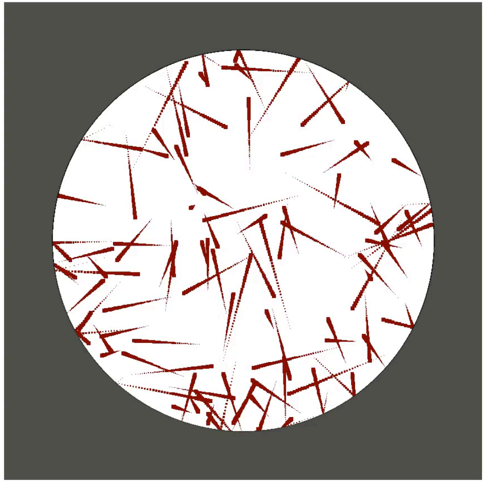
Random Walk Solver

- Particle method for solving diffusion
- Velocity and mean path for each particle based on exponential distribution
- Diffuse reflections are used for surface collisions
- Symmetric boundary conditions

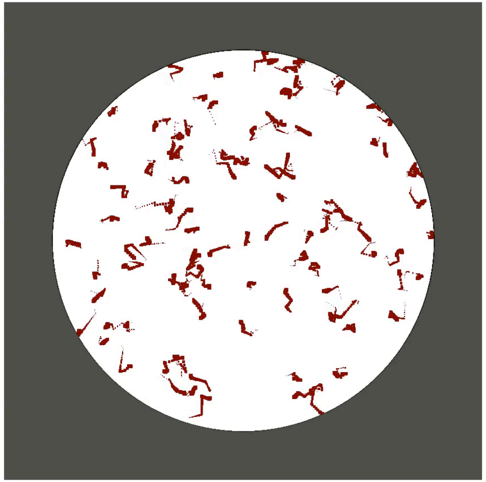
$$D_{eff_i} = \frac{\langle \xi^2 \rangle}{2t}$$

- $\langle \xi^2 \rangle$ is the mean square displacement of the particles

- Mean thermal velocity, $\bar{v}$, and mean free path, $\bar{\lambda}$, are imposed to simulate the desired gas species and conditions.



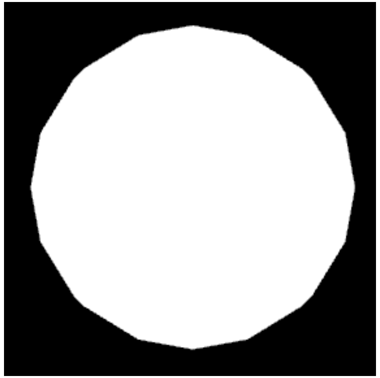
High Knudsen



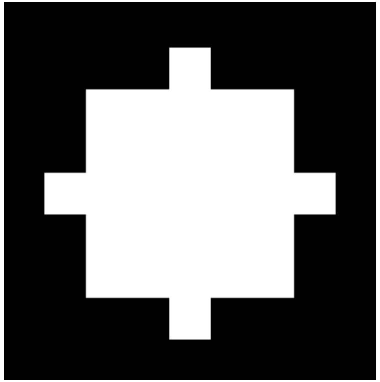
Low Knudsen

Wall Collisions

- Diffuse reflections used for surface collisions
- Collision detection can be based on isosurface or cuberille grid

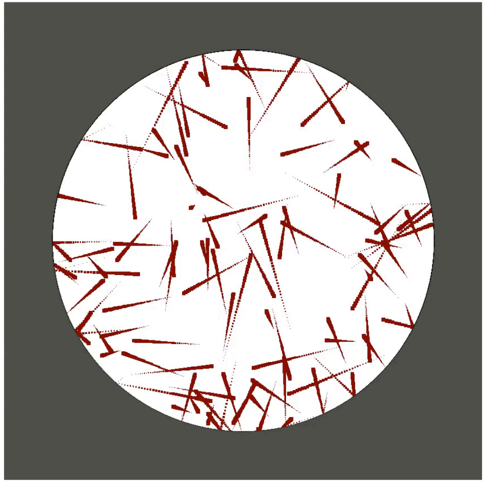


(a)

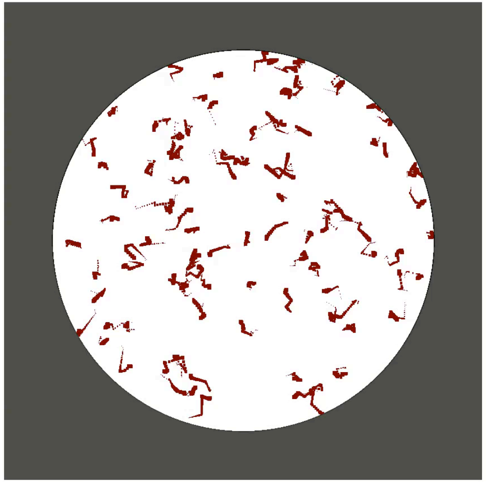


(b)

Isosurface (a) and cuberille (b) approximations of a cylinder with radius 3 voxels.



High Knudsen



Low Knudsen

Wall Collisions

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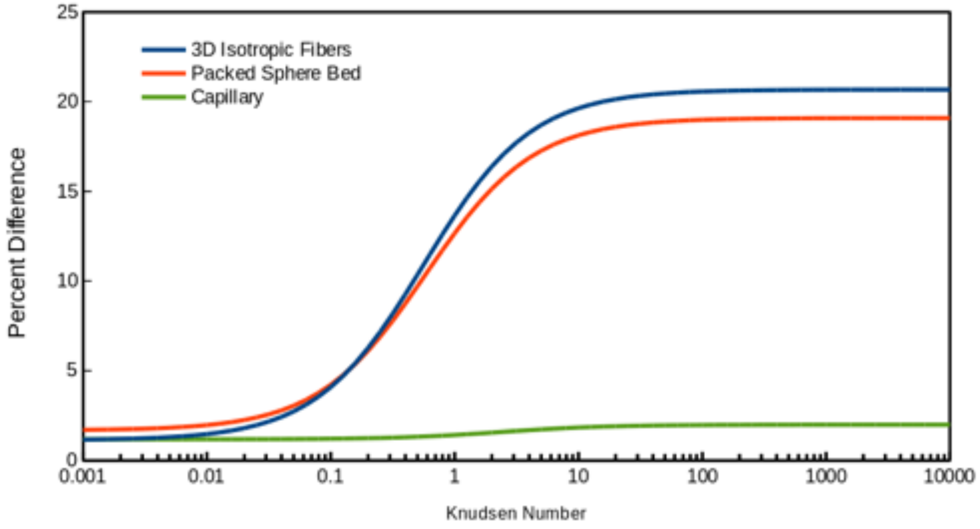
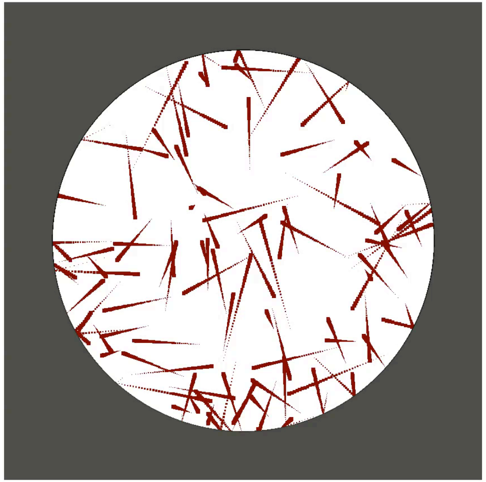
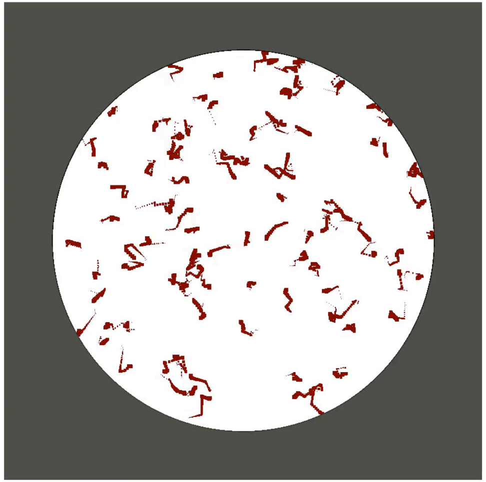


Percent difference (isosurface vs cuberille) vs Knudsen number for three different ideal geometries



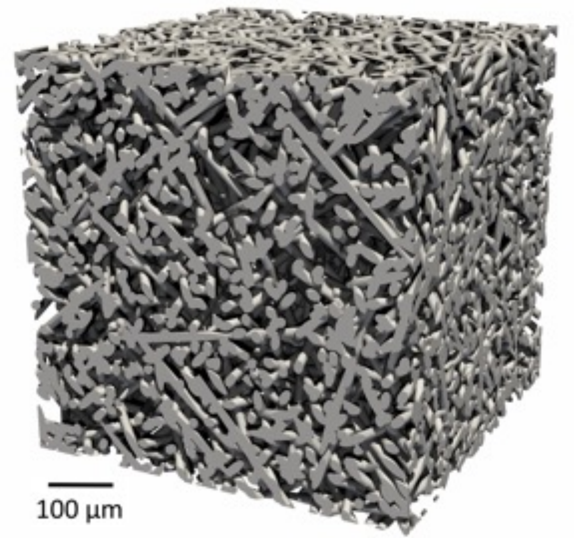
High Knudsen

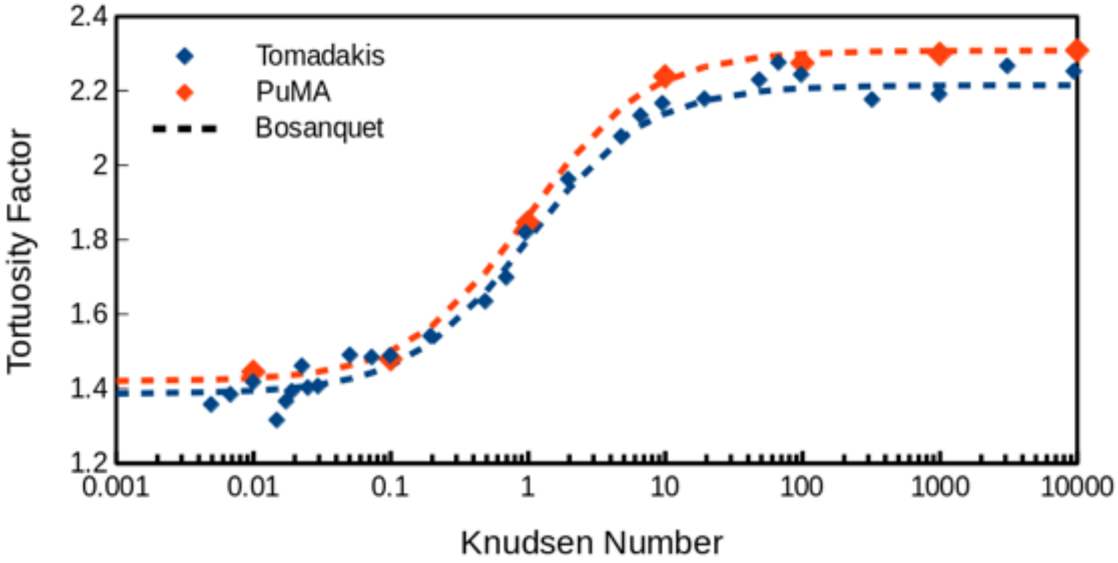


Low Knudsen

Comparison to Literature

Test Case #1



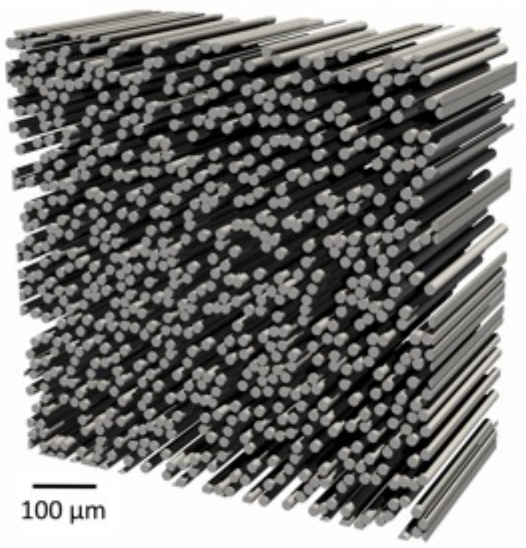


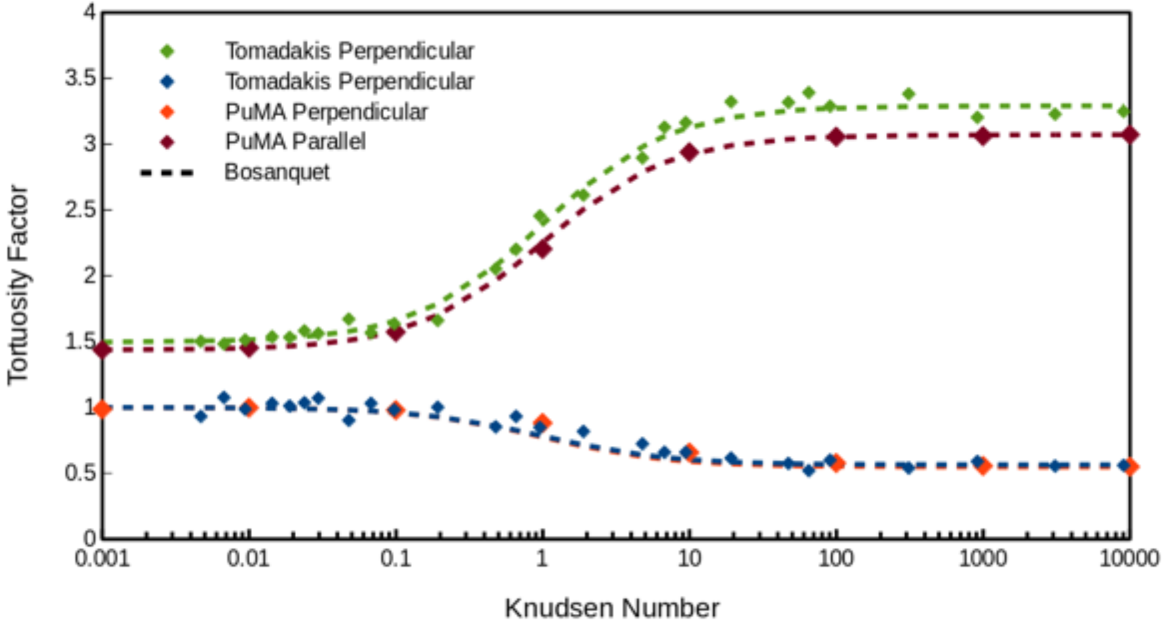
- 3D Fibers, 512^3
- Intersecting, isotropic
- 0.6 porosity

The 5% error is likely due to the limitations of computing in 1993. Simulations by Tomadakis were using only 200 particles and likely on a small dataset. The PuMA simulations were run on 200,000 particles for a total walk length of 10,000 times the domain length

Comparison to Literature

Test Case #2



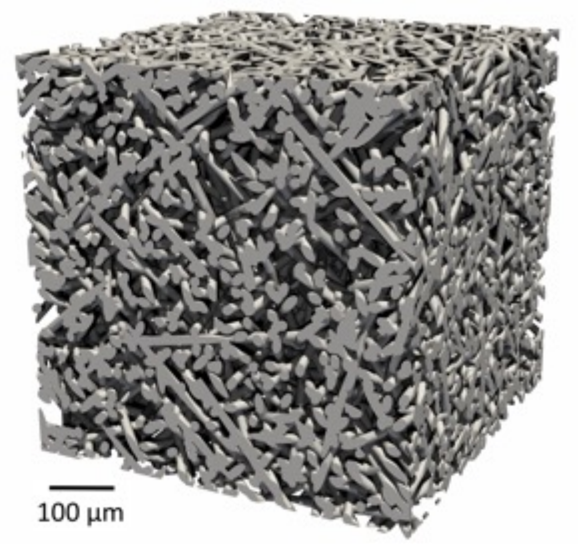


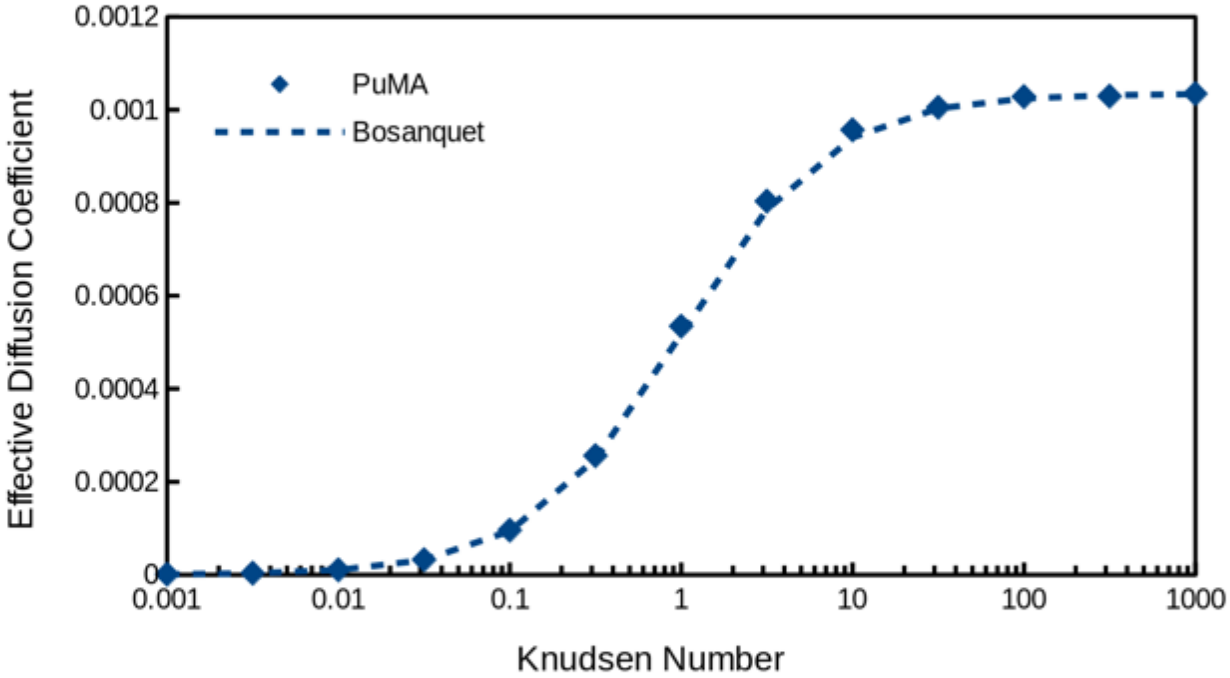
- 1D Fibers, 512 x 512 x 256
- Non intersecting
- 0.7 porosity

The 5% error is likely due to the limitations of computing in 1993. Simulations by Tomadakis were using only 200 particles and likely on a small dataset. The PuMA simulations were run on 200,000 particles for a total walk length of 10,000 times the domain length

Bosanquet Analysis

Test Case #1

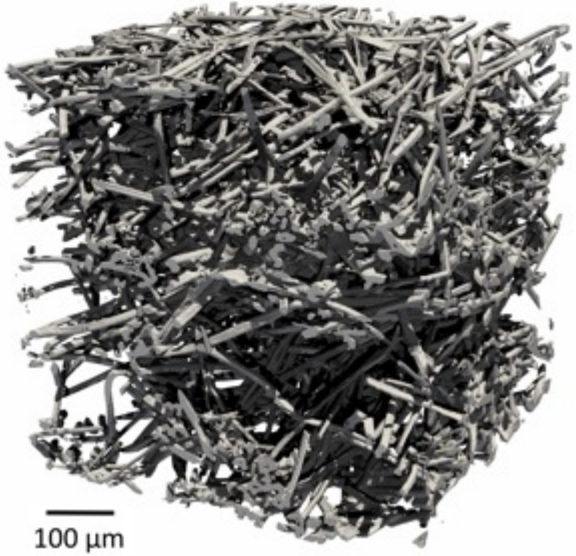




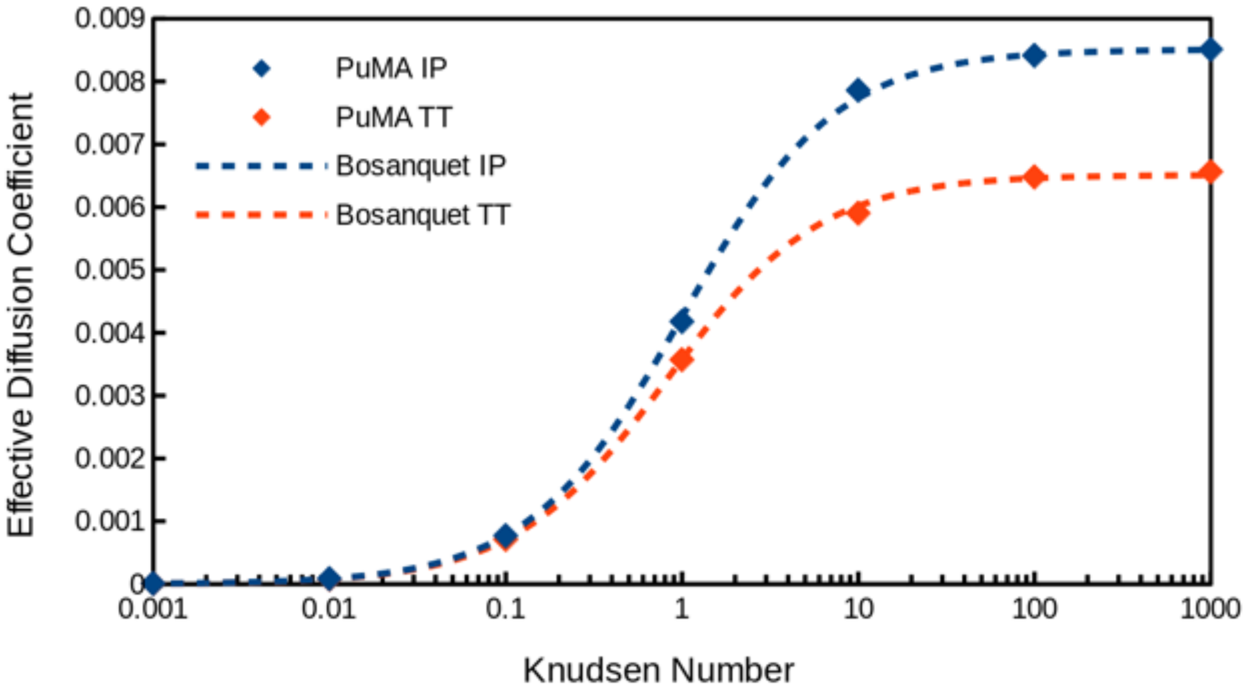
- 3D Fibers, 512^3
- Intersecting, isotropic
- 0.6 porosity

Bosanquet Analysis

Test Case #2



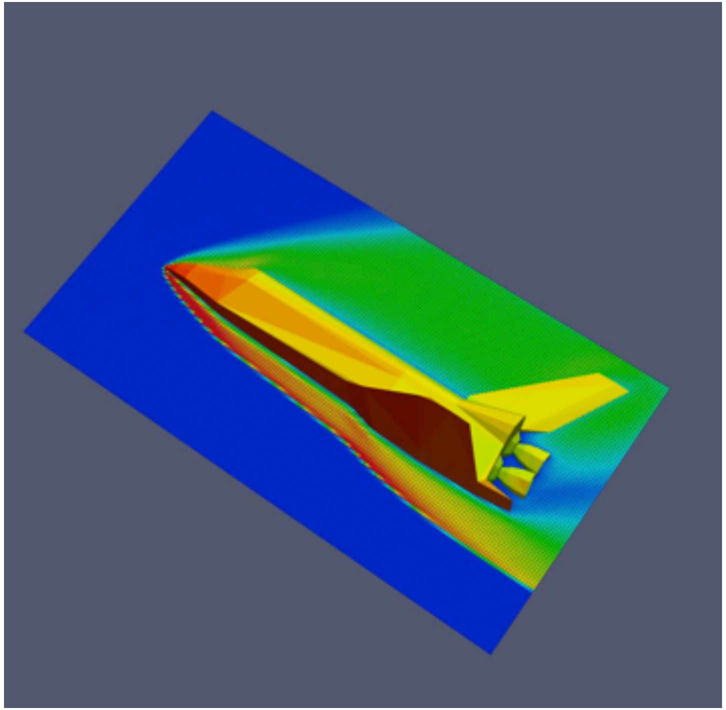
- FiberForm, 0.8 mm^3
- Transverse isotropic
- 0.89 porosity



Direct Simulation Monte Carlo

- DSMC is a particle method to simulate transitional and rarified flows with high fidelity
- Very computationally expensive, preventing large or frequent simulations
- DSMC diffusion simulations conducted in SPARTA, developed at Sandia National Labs.
- Pressure varied to change the mean free path, and therefore the Knudsen number

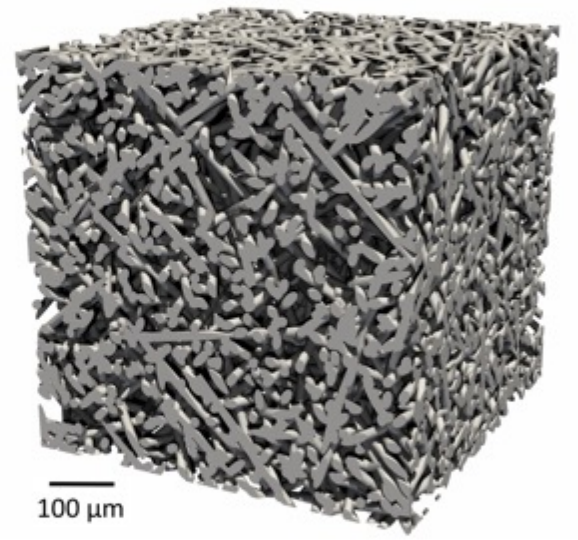
- **Used as a verification case for the random walk method**

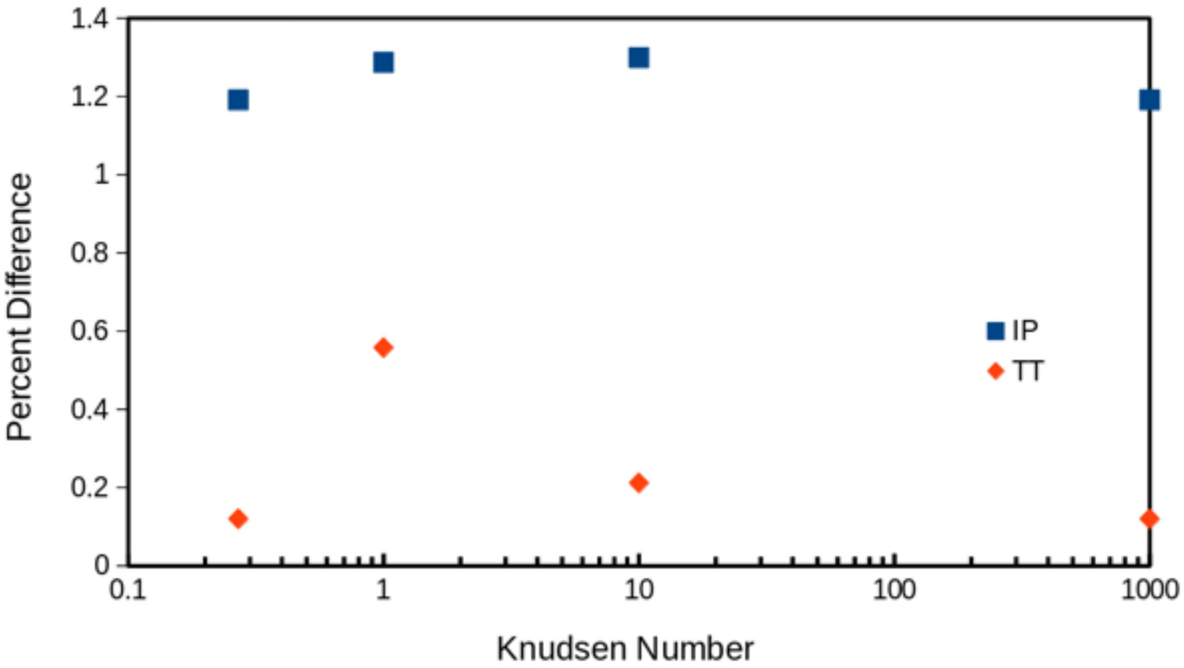


DSMC simulation of transitional flow over the Space Shuttle. Sparta.sandia.gov

Direct Simulation Monte Carlo

Test Case #1

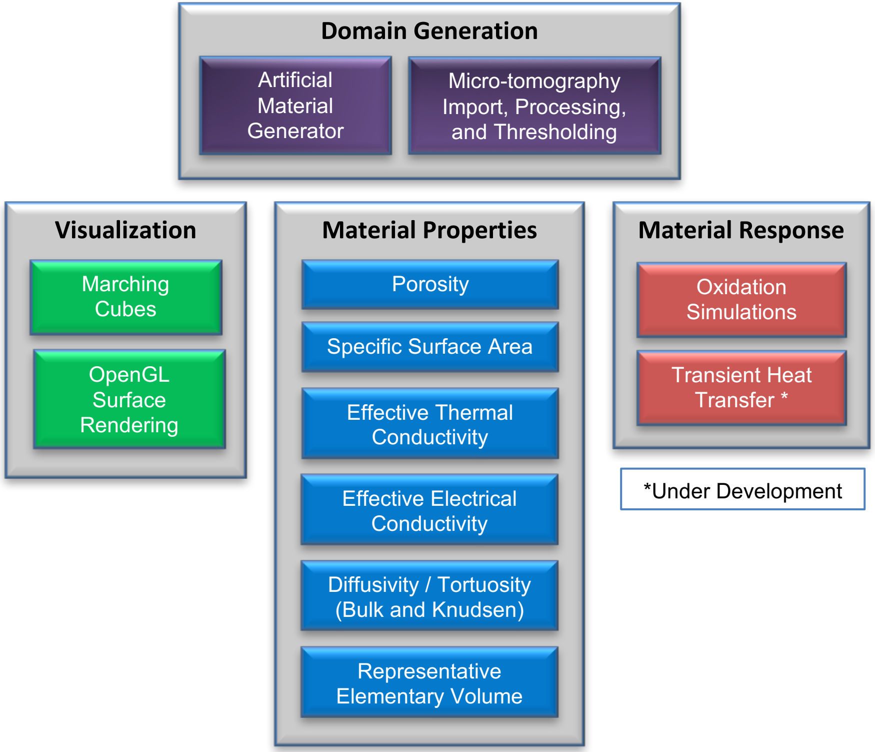




- 3D Fibers, 512^3
- Intersecting, isotropic
- 0.6 porosity

Conclusion and Outlook

- Implemented finite difference and random walk tortuosity factor solvers into PuMA V2.1
- Demonstrated the necessity of using an isosurface collision detection for complex 3d media, a capability which currently only exists in PuMA
- Verified random walk model for tortuosity factors against Direct Simulation Monte Carlo (DSMC) simulations.
- Recommend changing current definitions of tortuosity factor to restore the value as a purely geometrical property.



Acknowledgements

- This work was supported by the Entry System Modeling project (M.J. Wright project manager) of the NASA Game Changing Development program.

- T. Sandstrom, C. Henze, D. Ellsworth, and B. Nelson for useful discussions during the development of PuMA and the parallelization of the oxidation model.

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Questions?

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Ablation WS, 2017
Bozeman, MT